Agrochemical Analysis
by Photoionization MS

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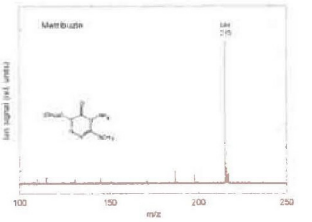

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Outline

- Problem
  - *Agrochemicals including pesticides are not routinely detectable by ESI and APCI*
  - *Chemical weapons have similar detection problems*
  - *This work evaluates the applicability of photoionization (PI) MS*
- Experimental
  - *Low pressure photoionization (LPPI) with quadrupole ion trap TOF (QitTof™) MS -- (Syagen Radiance Pro)*
  - *APPI and APCI with flow injection MS – (Agilent 1100 Series LC/MSD)*
- Results
  - *Comparison of LPPI to atmospheric pressure sources APPI and APCI*
  - *Detectability of CW agents and byproducts in soil extracts and contaminated water*
  - *Lessons learned*
- Conclusions

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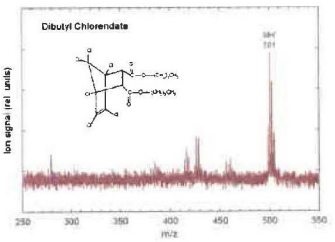
Chlorinated Pesticides: Non-aromatic vs. Aromatic

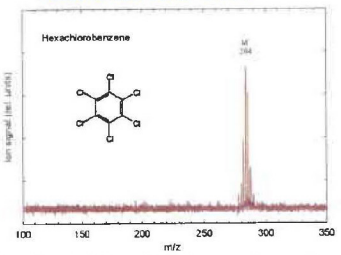
IP's of non-aromatic chlorinated cyclic hydrocarbons

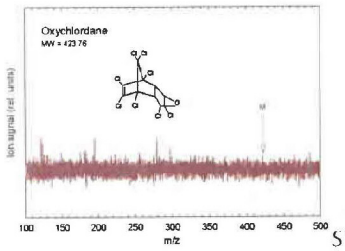
- Cyclohexane: IP = 9.88 eV
- Chlorocyclohexane: IP = 10.10 eV
- Hexachlorohexane (α-BHC): not observed
- Dibutyl Chlorendate: 10 < IP < 10.6 ???

IP's of highly chlorinated aromatics

- Benzene: IP = 9.24 eV
- Hexachlorobenzene: 9.0 eV







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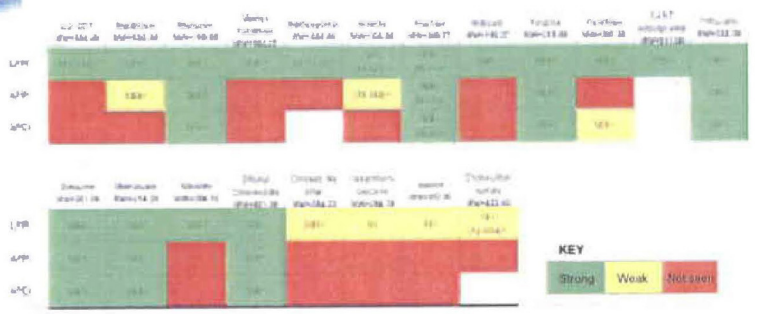
LPPI vs. APPI vs. APCI



Characteristics of compounds that photoionize

- Aromatics work well
- LPPI has higher detection rate than APPI, which in turn is moderately better than APCI

Other observations

- Ion dissociation efficient for compounds containing $-CCl_3$ (e.g. p,p'-DDT and methoxychlor)
- MH^+ detected for compounds with basic functional groups

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